EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	0	samsoondar.in. and james.in. and apperture	US-PGPUB; USPAT	OR	ON	2007/12/29 11:56
L2	7	samsoondar.in. and james.in. and aperture	US-PGPUB; USPAT	OR	ON	2007/12/29 11:57
L3	59	samsoondar.in. and james.in.	US-PGPUB; USPAT	OR	ON	2007/12/29 12:35
L4	4475	422/63-67,82.05-82.09,82.11.ccls.	USPAT	OR	ON	2007/12/29 12:36
L5	1471	4 and calibrat$	USPAT	OR	ON	2007/12/29 12:37
L6	553	422/58.ccls. and calibrat$	USPAT	OR	ON	2007/12/29 12:37
L7	1856	5 6	USPAT	OR	ON	2007/12/29 15:33
L8	228	bilirubin near6 interfer$	USPAT	OR	ON	2007/12/29 16:29
L9	192	8 and (photomet$ or colorimet$ or spectrophotomet$)	USPAT	OR	ON	2007/12/29 15:34
L10	57	8 and 422/55-104.ccls.	USPAT	OR	ON	2007/12/29 15:34
L11	118	8 and 436/1-183.ccls.	USPAT	OR	ON	2007/12/29 15:35
L12	203	9 10 11	USPAT	OR	ON	2007/12/29 16:05
L13	135	12 and(equation or calibrat? or formula or algorithm)	USPAT	OR	ON	2007/12/29 16:06
L14	154	8 and(equation or calibrat? or formula or algorithm)	USPAT	OR	ON	2007/12/29 16:06
L15	696	(hemoglobin or haemoglobin or bilirubin) near7 interfer$	USPAT	OR	ON	2007/12/29 16:30
L16	7	15 and sode$.xa,xp.	USPAT	OR	ON	2007/12/29 17:03

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=> d his

     (FILE 'HOME' ENTERED AT 17:09:41 ON 29 DEC 2007)
     FILE 'CA' ENTERED AT 17:09:55 ON 29 DEC 2007
L1   9993 S (COLORIMET? OR PHOTOMET? OR SPECTROPHOTOMET?)AND(CALIBRAT? OR
          MEASUR? OR OXIMET?)(5A)(FORMULA OR EQUATION OR ALGORITHM OR MODEL
          OR SIMULAT? OR METHOD)
L2  10079 S (COLORIMET? OR PHOTOMET? OR SPECTROPHOTOMET? OR OXIMET?)AND
          (CALIBRAT? OR MEASUR?)(5A)(FORMULA OR EQUATION OR ALGORITHM OR
          MODEL OR SIMULAT? OR METHOD)
L3   4271 S (TRANSFER? OR VALIDAT? OR BARCODE OR BAR CODE)(6A)(CALIBRAT? OR
          MEASUR?)(5A)(FORMULA OR EQUATION OR ALGORITHM OR MODEL OR SIMULAT?
          OR METHOD)
L4    104 S L1-2 AND L3
L5   3941 S (MULTI OR MULTIPLE OR PLURAL?)(2A)(INSTRUMENT OR ANALY!ER OR
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L6     37 S L1-2 AND L5
L7      8 S L3 AND L5
L8     85 S (COLORIMET? OR PHOTOMET? OR SPECTROPHOTOMET? OR OXIMET?)AND
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          (2A) STANDARDI?)
L9    573 S CALIBRAT?(3A)TRANSFER?
L10   105 S L9 AND(REGRESSION OR MULTIVARIATE OR CHEMOMET? OR GENETIC)
L11   344 S L3 AND(REGRESSION OR MULTIVARIATE OR CHEMOMET? OR GENETIC)
L12   209 S L10-11 AND(OPTIC? OR INFRARED OR NIR OR ULTRAVIOLET OR VISIBLE OR
          LIGHT OR LASER)
L13   406 S L4,L6-8,L12
L14   278 S L13 AND PY<2004
L15    23 S L13 AND PATENT/DT AND PY<2006
L16   282 S L14-15
L17   255 S L16 NOT(ATTENUATED TOTAL OR POLAROGRAP? OR SUPERNOVA OR WOOD OR
          DUST OR AEROSOL OR COMPOST OR RADIOMETER OR OPAL)
L18   226 S L17 NOT(BEETLE OR 1948/TI OR BAFFLE OR DISCHARGE OR HPLC OR ORE OR
          PERSEA OR BANDING OR HALFTONE OR PHOTOTHERM? OR PROPELLANT OR
          FLUORESCENT COLOURS)

=> d bib,ab 118 1-226
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L18   ANSWER 18 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   139:304090   CA
TI   **Multivariate** calibration standardization across instruments for the
      determination of glucose by Fourier transform near-**infrared** spectrometry
AU   Zhang, Lin; Small, Gary W.; Arnold, Mark A.
CS   Center for Intelligent Chemical Instrumentation, Department of Chemistry
      and Biochemistry, Clippinger Laboratories, Ohio University, Athens, OH,
      45701, USA
SO   Analytical Chemistry (**2003**), 75(21), 5905-5915
AB   The **transfer** of **multivariate calibration models** is investigated between
      a primary (A) and two secondary Fourier transform near-**IR** (near-**IR**)
      spectrometers (B, C). The application studied in this work is the use
      of bands in the near-**IR** combination region of 5000-4000 $cm-1$ to det.
      physiol. levels of glucose in a buffered aq. matrix contg. varying
      levels of alanine, ascorbate, lactate, triacetin, and urea. The three
      spectrometers are used to measure 80 samples produced through a

randomized exptl. design that minimizes correlations between the component concns. and between the concns. of glucose and water. Direct standardization (DS), piecewise direct standardization (PDS), and guided model reoptimization (GMR) are evaluated for use in **transferring** partial least-squares **calibration models** developed with the spectra of 64 samples from the primary instrument to the prediction of glucose concns. in 16 prediction samples measured with each secondary spectrometer. The three algorithms are evaluated as a function of the no. of standardization samples used in **transferring** the **calibration models**. Performance criteria for judging the success of the **calibration transfer** are established as the std. error of prediction (SEP) for internal calibration models built with the spectra of the 64 calibration samples collected with each secondary spectrometer. These SEP values are 1.51 and 1.14 mM for spectrometers B and C, resp. When calibration standardization is applied, the GMR algorithm is obsd. to outperform DS and PDS. With spectrometer C, the **calibration transfer** is highly successful, producing an SEP value of 1.07 mM. However, an SEP of 2.96 mM indicates unsuccessful calibration standardization with spectrometer B. This failure is attributed to differences in the variance structure of the spectra collected with spectrometers A and B. Diagnostic procedures are presented for use with the GMR **algorithm** that forecasts the successful **calibration transfer** with spectrometer C and the unsatisfactory results with spectrometer B.

L18   ANSWER 40 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   137:255002   CA
TI   New hybrid **algorithm** for **transferring multivariate** quantitative **calibrations** of intra-vendor near-**infrared** spectrometers
AU   Wehlburg, Christine M.; Haaland, David M.; Melgaard, David K.
CS   Sandia National Laboratories, Albuquerque, NM, 87185-0886, USA
SO   Applied Spectroscopy (**2002**), 56(7), 877-886
AB   A new prediction-augmented classical least-squares/partial least-squares (PACLS/PLS) hybrid algorithm is ideally suited for use in **transferring multivariate calibrations** between spectrometers. Spectral variations such as instrument response differences can be explicitly incorporated into the algorithm through the use of subset sample spectra collected on both spectrometers. Two current **calibration transfer methods**, subset recalibration and piecewise direct standardization (PDS), also use subset sample spectra to facilitate **transfer** of **calibration**. The three **methods** were applied to the **transfer** of quant. **multivariate calibration models** for near-**IR** (**NIR**) data of org. samples contg. chlorobenzene, heptane, and toluene between a primary and three secondary spectrometers that were all the same **model**, called intra-vendor **transfer** of **calibration**. The hybrid PACLS/PLS method outperformed subset recalibration and provided predictions equiv. to PDS with additive background correction on the two secondary spectrometers whose instrument drift appeared to be dominated by simple linear baseline variations. One of the secondary spectrometers had complex instrument drift that was captured by repeatedly measuring the spectrum of a single repeat sample. In calcg. a transfer function to correct prediction spectra, PDs assumes no instrumental drift on the secondary spectrometer. Therefore, PDS was unable to directly accommodate both the subset samples and the use of a single repeat sample to **transfer** and

maintain a **calibration** on that secondary instrument. In order to
implement the **transfer** of **calibration** with PDS in the presence of
complex instrument drift, recalibrated PLS models that included the
repeat spectra from the secondary spectrometer were used to predict the
spectra transformed by PDS. The importance of correcting for drift on
the secondary spectrometer during **calibration transfer** was illustrated
by the improvements in prediction for all three methods vs. using only
the instrument response differences derived from the subset sample
spectra. When the effects of instrument drift were complex on the
secondary spectrometer, the PACLS/PLS hybrid algorithm outperformed both
PDs and subset recalibration. Through the explicit incorporation of
spectral variations, due to instrument response differences and drift on
the secondary spectrometer, the PACLS/PLS **algorithm** was successful at
intra-vendor **transfer** of **calibrations** between **NIR** spectrometers.

L18 ANSWER 64 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   135:136557 CA
TI   **Calibration transfer** between PDA-based **NIR** spectrometers in the **NIR**
     assessment of melon soluble solids content
AU   Greensill, C. V.; Wolfs, P. J.; Spiegelman, C. H.; Walsh, K. B.
CS   Faculty of Engineering and Physical Systems, Central Queensland
     University, Rockhampton, 4702, Australia
SO   Applied Spectroscopy (**2001**), 55(5), 647-653
AB   In near-**IR** (**NIR**) spectroscopy, the transfer of predictive models between
     Fourier transform near-**IR** (FT-**NIR**) and scanning-grating-based
     instruments has been accomplished on relatively dry samples (<10% water)
     using various **chemometric** techniques-for example, slope and bias
     correction (SBC), direct standardization (DS), piecewise direct
     standardization (PDS), orthogonal signal correction (OSC), finite
     impulse transform (FIR) and wavelet transform (WT), and application of
     neural networks. In this study, seven well-known techniques [SBC, DS,
     PDS, double-window PDS (DWPDS), OSC, FIR, and WT], a **photometric**
     response correction and wavelength interpolative method, and a model
     updating method were assessed in terms of root mean square error of
     prediction (RMSEP) (using Fearn's significance testing) for **calibration**
     transfer (standardization) between pairs of spectrometers from a group
     of four spectrometers for noninvasive prediction of sol. solid content
     (SSC) of melon fruit. The spectrometers were diffraction grating-based
     instruments incorporating photodiode array photodetectors (MMS1, Carl
     Zeiss, Jena, Germany), used with a std. **optical** geometry of sample,
     light source, and spectrometer. A modified WT method performed
     significantly better than all other standardization methods and on a par
     with model updating.

L18 ANSWER 74 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   133:49006 CA
TI   Assessing the **transfer** of quantitative **NIR calibrations** from a
     spectrometer to another one
AU   Ulmschneider, M.; Penigault, E.
CS   Pharmaceutical Quality Control and Assurance, F. Hoffmann - La Roche
     Ltd, Basel, CH-4070, Switz.
SO   Analusis (**2000**), 28(1), 83-87
AB   Many factors account for the **optical** differences between two near-**IR**

(**NIR**) spectrometers of the same make and type. The use of two **NIR**
spectrometers may involve different **calibrations**, that can be
transferred only with addnl. work, like bias adjustments, other sample
measurements, model recalcns., conversion of spectral data, etc. In
most cases direct transfers of the applications are not possible. In
this study the feasibility of a **calibration transfer** between
FOSS/NIRSystems **NIR** spectrometers was checked. The set of **multivariate**
calibrations for a non-invasive identity testing and a direct detn. of
the water content in ceftriaxone disodium salt sterile (Rocephin) and in
a prepn. contg. tenoxicam active substance (Tilcotil) filled in vials,
was transferred from one spectrometer to another. Sep. bias adjustments
were calcd. for each calibration to fit the spectral data collected on
both instruments. These considerations define a practicable procedure
to transfer quant. **NIR** applications with a reasonable amt. of addnl.
work.

L18   ANSWER 75 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   132:356289 CA
TI   Adaptable **multivariate** calibration models for spectral applications
AU   Thomas, Edward V.
CS   Sandia National Laboratories, Albuquerque, NM, 87185-0829, USA
SO   Analytical Chemistry (**2000**), 72(13), 2821-2827
AB   **Multivariate** calibration techniques were used in a wide variety of
       spectroscopic situations. In many of these situations, spectral
       variation can be partitioned into sep. classes. For example, suppose
       that multiple spectra were obtained from each of a no. of different
       objects wherein the level of the analyte of interest varies within each
       object over time. In such situations, the total spectral variation
       obsd. across all measurements has two distinct general sources of
       variation: intraobject and interobject. One might want to develop a
       global **multivariate** calibration model that predicts the analyte of
       interest. accurately both within and across objects, including new
       objects not involved in developing the calibration model. However, this
       goal might be hard to realize if the interobject spectral variation is
       complex and difficult to model. If the intraobject spectral variation
       is consistent across objects, an effective alternative approach might be
       to develop a generic intraobject model that can be adapted to each
       object sep. This paper contains recommendations for exptl. protocols
       and data anal. in such situations. The approach is illustrated with an
       example involving the noninvasive measurement of glucose using near-**IR**
       reflectance spectroscopy. Extensions to **calibration** maintenance and
       calibration transfer are discussed.

L18   ANSWER 79 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   132:216257 CA
TI   Correction of temperature-induced spectral variation by continuous
       piecewise direct standardization
AU   Wuelfert, Florian; Kok, Wim Th.; de Noord, Onno E.; Smilde, Age K.
CS   Department of Chemical Engineering Process Analysis & Chemometrics,
       University of Amsterdam, Amsterdam, 1018 WV, Neth.
SO   Analytical Chemistry (**2000**), 72(7), 1639-1644
AB   In process anal. applications it is not always possible to keep the
       measurement conditions const. However, fluctuations in external

variables such as temp. can have a strong influence on measurement results. For example, nonlinear temp. effects on near-**IR** (**NIR**) spectra may lead to a strongly biased prediction result from **multivariate** calibration models such as PLS. A new method, called Continuous Piecewise Direct Standardization (CPDS) was developed for the correction of such external influences. It represents a generalization of the discrete PDS **calibration transfer method** and is able to adjust for continuous nonlinear influences such as the temp. effects on spectra. It was applied to short-wave **NIR** spectra of ethanol/water/2-propanol

mixts. measured at different temps. in the range 30-70°. The method was able to remove, almost completely, the temp. effects on the spectra, and prediction of the mole fractions of the chem. components was close to the results obtained at const. temp.

L18   ANSWER 95 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   130:257423   CA
TI   **Multi-instrument** calibration with **genetic regression** in **UV-visible** spectroscopy
AU   Ozdemir, Durmus; Williams, Ron
CS   Department of Chemistry Hunter Laboratories, Clemson University, Clemson, SC, 29634, USA
SO   Applied Spectroscopy (**1999**), 53(2), 210-217
AB   The applicability of **genetic regression** (GR) to **multi-instrument** calibration was demonstrated by using several **UV-visible spectrophotometers**. GR is a calibration technique that optimizes linear **regression** using a **genetic** algorithm (GA). Sample spectra of ternary and quaternary mixts. of the pharmaceuticals furaltadone (Fd), doxycycline (Dx), sulfadiazine (Sd), and trimethoprim (Tm) were collected on four different **UV-visible spectrophotometers**, including one single-beam diode array and three double-beam dispersive instruments. Hybrid **calibration models** (HCMs) were generated by combining the data collected on **multiple instruments** into one **calibration model** as if they had all been collected on a single instrument. For comparison, single-instrument **calibration models** were also generated for each instrument. Both HCMs and single-instrument **models** were tested by using a **validation** set **measured** on all four instruments. Results obtained from single-instrument models were comparable with a previous study in which partial least squares (PLS) **regression** was used for **multivariate** calibration of these compds. HCMs for double-instrument cases performed equally well as single-instrument models and slightly worse for the four-instruments models.

L18   ANSWER 96 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   130:222296   CA
TI   Simultaneous **spectrophotometric** determination of tartrazine, patent blue V, and indigo carmine in commercial products by partial least squares and principal component **regression** methods
AU   Nevado, J. J. Berzas; Flores, J. Rodriguez; Llerena, M. J. Villasenor; Farinas, N. Rodriguez
CS   Department of Analytical Chemistry and Food Technology, University of Castilla-La Mancha, Ciudad Real, 13071, Spain
SO   Talanta (**1999**), 48(4), 895-903

AB   Two **multivariate calibration methods**, partial least squares (PLS-1) and principal component **regression** (PCR) are proposed and successfully applied to the simultaneous detn. of three dyes, tartrazine (T) (E-102), patent blue V (P) (E-131), and indigo carmine (I) (E-132) in mixts. by **UV-visible** absorption **spectrophotometry**. **Calibration models** were evaluated by internal **validation** (prediction of dyes concn. in its own designed training set of calibration), by cross-validation (obtaining statistical parameters that show the efficiency for a **calibration** fit **model**), and by external **validation** over 19 synthetic mixts. of the three dyes in different ratios contg. 2.4-17.6 mg L-1 of T, 1.6-5.6 mg L-1 of P, and 3.2-17.5 mg/1-1 of I, with recoveries between 93.5 and 103.1% and over three com. products, in which the proposed **calibration models** were satisfactorily applied without sepn. step. Repeatability and reproducibility studies (with the Students's and F tests) were achieved over two series of nine stds. for each dye, showing no significant differences at 95% confidence level.

L18   ANSWER 100 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   130:133393 CA
TI   An evaluation of orthogonal signal correction applied to **calibration transfer** of near **infrared** spectra
AU   Sjoblom, Jonas; Svensson, Olof; Josefson, Mats; Kullberg, Hans; Wold, Svante
CS   Analytical Chemistry, Pharmaceutical R&D, Astra Hassle AB, Moelndal, S-431 83, Swed.
SO   Chemometrics and Intelligent Laboratory Systems (**1998**), 44(1,2), 229-244
AB   Orthogonal signal correction (OSC) is a technique for preprocessing of, for example, **NIR**-spectra before they are subjected to a **multivariate** calibration. With OSC the X-matrix is cor. by a subtraction of variation that is orthogonal to the calibration Y-matrix. This correction can then be applied to new spectra that are going to be used in predictions. The aim of this study is to study if the OSC transform makes the spectra less dependent of instrument variation. This may result in easier **calibration model transfer** between different instruments without creating or re-analyzing the whole calibration sample set. OSC was applied to **NIR**-spectra that were used in a calibration for the water content in a pharmaceutical product. Partial least squares calibrations were then compared to other calibration models with uncorrected spectra, models with spectra subjected to multiplicative signal correction, and a no. of other transfer methods. The performance of OSC was on the same level as for piece-wise direct standardization and spectral offset correction for each individual instrument and PLS-models with both instruments included.

L18   ANSWER 101 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   129:267675 CA
TI   Method for standardizing Raman spectrometers to obtain stable and **transferable calibrations**
IN   Carman, Howard S., Jr.; Alsmeyer, Daniel C.; Huarez-Garcia, Carlos Humberto; Garrett, Aaron W.; Wilson, Bruce E.; Nicely, Vincent A.
PA   Eastman Chemical Co., USA
SO   PCT Int. Appl., 58 pp.
PI   **WO 9841825**   **A1**   **19980924**   **WO 1998-US4321**   **19980305**

US 5850623   **A**   **19981215**   **US 1997-947689**   **19971009**
PRAI US 1997-43588P   P   19970314
      US 1997-947689   A   19971009

AB   Methods for providing an accurate and precise quant. anal. of the chem. compn. and/or phys. properties of an unknown sample use the std. Raman spectra of a plurality of known samples to construct a normalized calibration, which is applied to a std. Raman spectrum of the unknown sample obtained from a particular Raman spectrometry app. or any similar Raman spectrometry app., which is used to simultaneously irradiate a ref. material and at least one sample, thereby obtaining their resp. convolved Raman spectra. Using a defined std. energy dispersion characteristic and a std. Raman spectrum of the ref. material, a convolved function is detd. and applied to produce a deconvolved Raman spectrum of the sample. This deconvolved spectrum is multiplied by a defined std. **photometric** response function to produce a std. Raman spectrum of the sample, thereby providing an accurate and precise quant. anal. The process may be repeated using a plurality of std. samples to produce a multivariate signal response set from which a normalized calibration which may then be applied to unknown samples.

L18   ANSWER 106 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   129:117171   CA
TI   Standardization of fiber-**optic** probes for near-**infrared multivariate** calibrations
AU   Sum, Stephen T.; Brown, Steven D.
CS   Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716, USA
SO   Applied Spectroscopy (**1998**), 52(6), 869-877
AB   The standardization of Fourier transform near-**IR** (FT-**NIR**) spectrometers equipped with fiber-**optic** probes was studied. FT-**NIR** spectra of caustic brines for an industrial process were measured on two different instruments. **Calibration transfer** across the instruments and probes was studied by employing calibration models built on one instrument to predict properties from spectra measured on the other. The transfer was examd. by using spectra without and with preprocessing. The preprocessing methods included a Savitzky-Golay (SG) deriv. polynomial filter, a procedure based on a finite impulse response (FIR) filter, and a combination of both. In addn. to being a preprocessing technique, the FIR filter is also a standardization method that transforms the instrument response function of one instrument to match that of another. The transformation was performed over a moving processing window without the use of transfer stds. Application of the FIR filter to 1st-deriv. spectra provided the best **multivariate calibration models** and led to the successful **transfer** of **calibration** across different probes and spectrometers.

L18   ANSWER 108 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   129:35727   CA
TI   **Transfer** of **calibrations** of near-**infrared** spectra using neural networks
AU   Despagne, Frederic; Walczak, Beata; Massart, Desire-Luc
CS   ChemoAC, Pharmaceutical Inst., Vrije Univ. Brussel, Brussels, B-1090, Belg.
SO   Applied Spectroscopy (**1998**), 52(5), 732-745

AB   A new approach for **multivariate** instrument standardization is presented.
     This approach is based on the use of neural networks (NNs) for modeling
     spectral differences between two instruments. In contrast to the
     piecewise direct standardization (PDS) method to which it is compared,
     the proposed method builds a single transfer model for all spectral
     windows. The apparently incompatible requirements for a high no. of
     training objects and a low no. of standardization samples are addressed
     by truncating spectra in finite-size windows and assessing a position
     index to each window. Each spectral window with the corresponding
     position index constitutes a training object. No prior background
     correction is required with this method. Both the proposed method and
     PDS were applied to some real and simulated data sets, and results were
     evaluated for reconstruction and subsequent calibration. On the studied
     data sets, the neural network approach was found to perform at least as
     well as PDS for both reconstruction and calibration.

AN   128:330544   CA
TI   Hybrid **calibration models**: an alternative to **calibration transfer**
AU   Ozdemir, Durmus; Mosley, Matt; Williams, Ron
CS   Dep. Chem., Clemson Univ., Clemson, SC, 29634, USA
SO   Applied Spectroscopy (**1998**), 52(4), 599-603
AB   A new procedure for calibrating **multiple instruments** is presented in
     which spectra from each were used simultaneously during the construction
     of **multivariate** calibration models. The application of partial least-
     squares (PLS) and **genetic regression** (GR) to the problem of generating
     these hybrid calibrations is presented. Spectra of ternary mixts. of
     methylene chloride, Et acetate, and methanol were collected on a
     dispersive and a Fourier transform spectrometer. Calibration models
     were generated by using differing nos. of spectra from each instrument
     simultaneously in the calibration and prediction sets, and then
     validated by using a set of spectra from each instrument sep.
     Calibration models were found that perform well on both instruments,
     even when only a single spectrum from the 2nd instrument was used during
     the calibration process. As a benchmark, comparison with PLS showed
     that GR is more effective than PLS in building these hybrid calibration
     models.

AN   128:188094   CA
TI   Comparison of two different approaches toward model transferability in
     NIR spectroscopy
AU   Swierenga, H.; Haanstra, W. G.; de Weijer, A. P.; Buydens, L. M. C.
CS   Laboratory Analytical Chemistry, Faculty Science, Catholic University
     Nijmegen, Nijmegen, 6525 ED, Neth.
SO   Applied Spectroscopy (**1998**), 52(1), 7-16
AB   Recently, efficient **methods** have become available to **transfer** a
     multivariate calibration model from one instrument to another. Two
     categories can be distinguished: improvement of the robustness of the
     calibration model by, for example, proper data preprocessing; and
     adaptation of the calibration model by, for example, (piecewise) direct
     standardization. In direct standardization, a subset from the
     calibration set should be measured on both instruments. Usually,

however, the calibration samples cannot be measured on both instruments. When data preprocessing is applied to the **transfer** of **multivariate calibration models**, there is no need for remeasurement of a subset on both instruments. In this paper, both categories are compared for the detn. of the component concns. in a ternary mixt. of methanol, ethanol, and 1-propanol using **NIR** spectroscopy. The **calibration models** obtained on one instrument are **transferred** to other **NIR** instruments. It has been found that the results of proper data preprocessing are comparable with the results obtained by direct standardization when the models are transferred over three **NIR** instruments.

L18   ANSWER 117 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   127:256772   CA
TI   **Calibration transfer** from a scanning near-**IR spectrophotometer** to a FT-near-**IR spectrophotometer**
AU   Lin, Jie; Lo, Su-Chin; Brown, Chris W.
CS   Department of Chemistry, Portland State University, Portland, OR, 97207-0751, USA
SO   Analytica Chimica Acta (**1997**), 349(1-3), 263-269
AB   A principal component **regression** calibration model developed on a scanning near-**IR spectrophotometer** (with a std. cuvette) was transferred to a Fourier transform near-**IR spectrophotometer** (with a fiber-**optic** probe) for the detn. of NaCl in aq. solns. by using piecewise direct standardization method. Only two transfer samples were needed in obtaining a good **calibration transfer**. Std. error of prediction obtainable from the **calibration transfer** was 0.034 M, compared to 0.012 M produced by the full set recalibration for NaCl in the concn. range of 0-5 M.

L18   ANSWER 118 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   127:247684   CA
TI   Applications of maximum likelihood principal component analysis: incomplete data sets and **calibration transfer**
AU   Andrews, Darren T.; Wentzell, Peter D.
CS   Trace Analysis Research Centre, Department of Chemistry, Dalhousie University, Halifax, NS, B3H4J3, Can.
SO   Analytica Chimica Acta (**1997**), 350(3), 341-352
AB   The application of a new method to the **multivariate** anal. of incomplete data sets is described. The new method, called max. likelihood principal component anal. (MLPCA), is analogous to conventional principal component anal. (PCA), but incorporates measurement error variance information in the decompn. of **multivariate** data. Missing measurements can be handled in a reliable and simple manner by assigning large measurement uncertainties to them. The problem of missing data is pervasive in chem., and MLPCA is applied to three sets of exptl. data to illustrate its utility. For exploratory data anal., a data set from the anal. of archeol. artifacts is used to show that the principal components extd. by MLPCA retain much of the original information even when a significant no. of measurements are missing. Maximum likelihood projections of censored data can often preserve original clusters among the samples and can, through the propagation of error, indicate which samples are likely to be projected erroneously. To demonstrate its utility in modeling applications, MLPCA is also applied in the

development of a model for chromatog. retention based on a data set which is only 80% complete. MLPCA can predict missing values and assign error ests. to these points. Finally, the problem of **calibration transfer** between instruments can be regarded as a missing data problem in which entire spectra are missing on the 'slave' instrument. Using **NIR** spectra obtained from two instruments, it is shown that spectra on the slave instrument can be predicted from a small subset of **calibration transfer** samples even if a different wavelength range is employed. Concn. prediction errors obtained by this approach were comparable to cross-validation errors obtained for the slave instrument when all spectra were available.

L18   ANSWER 122 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   127:114669 CA
TI   **Calibration transfer** from sample cell to fiber-**optic** probe
AU   Chen, Chi-Shi; Brown, Chris W.; Lo, Su-Chin
CS   Dep. Chem., Univ. Rhode Island, Kingston, RI, 02881-0809, USA
SO   Applied Spectroscopy (**1997**), 51(5), 744-748
AB   A **calibration transfer method**, piecewise direct standardization (PDS), was applied to a set of two-component samples measured on the same **UV-visible** spectrometer using a cuvette cell with a 10-mm path length and a fiber-**optic** probe with a 2-mm path length. Piecewise direct standardization proceeds by detg. a structured transformation matrix using the spectra of a few samples measured with both devices. This transformation matrix can then be used to transform any spectrum measured on one device to that obtained on another device, thereby making the **calibration model transferable** between devices. The authors used the spectra measured in a cuvette as the std. set and **transferred** the **calibration model** obtained for these spectra to spectra measured with a 2-mm fiber-**optic** probe on the same instrument. The total std. error of prediction (SEP) for the fiber-**optic** probe was 5.84 before the **calibration transfer** and 1.87 afterwards. Spectra were also processed by taking the Fourier transform prior to the **calibration transfer**. The 512 data points in each spectrum were compressed to 32 terms, starting with the 1st term after the d.c. offset. This processing reduced the background and the noise. As a consequence, in the Fourier domain, the total SEP was 5.69 before the calibration standardization and 0.79 after the calibration standardization. A **calibration transfer** was also performed between two fiber-**optic** probes; the total SEP in the spectral domain was 2.16 prior to the transfer and 1.04 after the transfer, whereas in the Fourier domain the SEP was 1.50 prior to the transfer and 0.77 after the transfer.

L18   ANSWER 132 OF 226 CA COPYRIGHT 2007 ACS on STN
AN   125:184432 CA
TI   Transfer of Near-**Infrared Multivariate** Calibrations without Standards
AU   Blank, Thomas B.; Sum, Stephen T.; Brown, Steven D.; Monfre, Stephen L.
CS   Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716, USA
SO   Analytical Chemistry (**1996**), 68(17), 2987-2995
AB   A novel approach to the **transfer** of **multivariate calibration** is proposed. This method is based on the finite impulse response (FIR)

filtering of a set of spectra to be transferred, using a spectrum on the target instrument to direct the filtering process. Often, the target spectrum is the mean of a calibration set. The method is compared against direct transfer and piecewise direct transfer on near-**IR** reflectance spectra in two representative data sets. Results from these studies suggest that FIR transfer compares favorably with piecewise direct transfer in terms of accuracy and precision of the match of **transferred** spectra to the predictive **calibration models** developed on the target instrument. Unlike piecewise direct transfer, FIR transfer requires no measurement of std. samples on both the source and target spectrometers. Details and current limitations of the FIR transfer method are presented.

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L18   ANSWER 134 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN    124:212175   CA
TI    Near-IR Detection of Polymorphism and Process-Related Substances
AU    Aldridge, P. K.; Evans, C. L.; Ward, H. W., II; Colgan, S. T.; Boyer,
      N.; Gemperline, P. J.
CS    Analytical Research and Development, Pfizer Central Research, Groton,
      CT, 06340, USA
SO    Analytical Chemistry (1996), 68(6), 997-1002
AB    A fast, sensitive pattern recognition method is reported for detg. the
      polymorphic quality of a solid drug substance, polymorph A. The pattern
      recognition method employed can discriminate between the desired
      polymorphic form of the drug substance and another undesired polymorph.
      In addn., it can reliably detect samples contg. minor levels of the
      undesired polymorph. The method can also discriminate between the
      desired polymorph and other cryst. forms. Most significantly, this
      sensitive method was successfully transferred to 6 other near-IR
      instruments without resorting to sophisticated multivariate calibration
      transfer strategies.
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L18   ANSWER 140 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN    123:357916   CA
TI    Calibration transfer for analytical instruments
IN    Kowalski, Bruce R.; Veltkamp, David J.; Wang, Yong D.
PA    University of Washington, USA
SO    U.S., 20 pp. Cont.-in-part of U.S. Ser. No. 595, 458, abandoned.
PI    US 5459677        A      19951017   US 1991-720256        19910624
      US 5559728        A      19960924   US 1994-237368        19940503
PRAI  US 1990-595458    B2     19901009
      US 1991-720256    A2     19910624
AB    A technique for transferring a multivariant calibration model from a
      ref. anal. instrument to a target anal. instrument that may be a
      different instrument, or the same instrument at a later time. In a
      ''direct'' approach, a plurality of transfer samples are selected, and a
      plurality of measurements are made for each transfer sample using the
      ref. instrument, producing a ref. instrument response for each sample.
      These measurements are repeated for the target instrument, to produce a
      target instrument response for each transfer sample. One then generates
      transfer coeffs. capable of performing a multivariate estn. of the ref.
      instrument responses for the transfer samples from the target instrument
      responses for those samples. The transfer coeffs. may then be used to
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convert a target instrument response for an unknown sample into the
equiv. response for the ref. instrument. In an important ''piecewise''
variation, the transfer coeffs. comprise a plurality of estn. coeffs.
for estg. each ref. data value from more-than-one but less-than-all
target data values. ''Classical'' and ''inverse'' transfer techniques
are also described, wherein target instrument responses for the transfer
samples are combined with ref. instrument responses for the full set of
calibration samples, to derive a multivariate prediction model for the
target instrument.

L18   ANSWER 141 OF 226 CA   COPYRIGHT 2007 ACS on STN
AN   123:328487 CA
TI   Modified Algorithm for Standardization of Near-**Infrared** Spectrometric
       Instruments
AU   Bouveresse, E.; Massart, D. L.; Dardenne, P.
CS   Pharmaceutical Institute, Vrije Universiteit Brussel, Brussels, Belg.
SO   Analytical Chemistry (**1995**), 67(8), 1381-9
AB   The **transfer** of **calibration models** between near-**IR** spectrometric
       instruments with the algorithm proposed by Shenk and Westerhaus as a
       standardization method is studied. This algorithm does not yield
       optimal results when standardization samples are used that are not of
       the same nature as the samples to be analyzed. In an attempt to improve
       the results obtained with this algorithm when one uses such
       standardization samples, five different modifications of the spectral
       intensity correction step of the algorithm are studied. The use of
       locally weighted **regression,** which gives more wt. to the standardization
       samples close to the same spectral intensity range where the samples to
       be predicted are located and less wt. to the farthest samples, seems to
       be the most suitable one.

L18   ANSWER 143 OF 226 CA   COPYRIGHT 2007 ACS on STN
AN   123:167901 CA
TI   A rapid, automated method for the determination of cis and trans content
       of fats and oils by Fourier transform **infrared** spectroscopy
AU   van de Voort, F. R.; Ismail, A. A.; Sedman, J.
CS   Dep. Food Science Agricultural Chemistry, Macdonald Campus of McGill
       Univ., St. Anne Bellevue, QC, H9X 3V9, Can.
SO   Journal of the American Oil Chemists' Society (**1995**), 72(8), 873-80
AB   A rapid Fourier transform **IR** (FTIR) method was developed to
       simultaneously det. percent cis and trans content of edible fats and
       oils. A generalized, industrial sample-handling platform/accessory was
       designed for handling both fats and oils and was incorporated into an
       FTIR spectrometer. The system was calibrated to predict the cis and
       trans content of edible oils by using pure triglycerides as stds. and
       partial least squares as the **chemometric** approach. The efficacy of the
       calibration was assessed by triglyceride std. addn., by mixing of oils
       with varying cis/trans contents, and by analyzing fats and oils of known
       iodine value. Each of the approaches verified that the FTIR method

       measured the cis and trans content in a reproducible (±0.7%) manner,
       with the measured accuracies being 1.5% for std. addn. and 2.5% for the
       chem. analyzed samples. Comparisons also were made to the conventional
       American Oil Chemists' Society (AOCS) method for the detn. of trans
       isomers by **IR** spectroscopy. The FTIR-partial least squares approach

worked well over a wide range of trans contents, including those between 0 and 15%. The sample-handling accessory designed for this application is robust, flexible, and easy to use, being particularly suited for quality-control applications. In addn., the anal. was automated by programming the spectrometer in Visual Basic (Windows), to provide a simple, prompt-based user interface and to allow an operator to carry out cis/trans analyses without any knowledge of FTIR spectroscopy. A typical anal. requires less than two minutes per sample. The derived **calibration** is **transferable** between instruments, eliminating the need for recalibration. The integrated anal. system provides a sound basis for the implementation of FTIR methods in place of a variety of AOCS wet chem. methods when anal. speed, cost, and environmental concerns are issues.

L18 ANSWER 144 OF 226 CA COPYRIGHT 2007 ACS on STN
AN 123:131613 CA
TI Additive Background Correction in **Multivariate** Instrument Standardization
AU Wang, Ziyi; Dean, Thomas; Kowalski, Bruce R.
CS Center for Process Analytical Chemistry, University of Washington, Seattle, WA, 98195, USA
SO Analytical Chemistry (**1995**), 67(14), 2379-85
AB Nonideal instruments give responses that do not follow Beer's law. Most spectrometers have some component of stray **light** that adds a structured, rather than const. or linear, background to absorbance spectra. When instrument standardization is performed using the multiplicative model introduced by Wang et al. (Anal. Chem. 1991, 63, 2750), the model does not explicitly include the additive term. This term, if uncorrected, can cause **multivariate** standardization to provide an incomplete **transfer** of **calibration models** between instruments. Using both simulation and real data, the current paper demonstrates the effect of the additive background term in **multivariate** standardization and provides an effective means by which such additive differences can be cor.

L18 ANSWER 146 OF 226 CA COPYRIGHT 2007 ACS on STN
AN 123:20869 CA
TI Wavelength **calibration transfer** between diode array **UV-visible spectrophotometers**
AU Blanco, Marcelo; Coello, Jordi; Iturriaga, Hortensia; Maspoch, Santiago; Rovira, Esther
CS Dep. Quimica, Universidad Autonoma Barcelona, Bellaterra, E-08193, Spain
SO Applied Spectroscopy (**1995**), 49(5), 593-7
AB The need to obtain expeditious results in control analyses of complex mixts. has turned **multivariate** calibration procedures into major choices for routine analyses. The inherent complexity of the calibration process and the practical need for analyses to be carried out as near the manufg. line as possible occasionally entail calibrating with a different instrument from that subsequently employed for the anal. measurements proper. This paper exposes the problems potentially arising in **transferring calibrations** between diode array **UV-visible spectrophotometers**. Basically, such problems originate in wavelength differences between **spectrophotometers**, even if they meet the manufacturer's specifications and the pharmacopoeia recommendations.

The authors developed a straightforward method for harmonizing instrumental responses from ref. wavelengths corresponding to zero values in the 1st-deriv. spectra for K dichromate and HOBz stds. The method was applied to the anal. of binary mixts. of theophylline and doxylamine by multiple linear and partial least-squares **regression** using one **spectrophotometer** for calibration and four others for analyses.

L18   ANSWER 147 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   122:158899   CA
TI   **Transfer** of **calibration** function in near-**infrared** spectroscopy
AU   Forina, M.; Drava, G.; Armanino, C.; Boggia, R.; Lanteri, S.; Leardi,
       R.; Corti, P.; Conti, P.; Giangiacomo, R.; et al.
CS   Istituto di Analisi e Tecnologie Farmaceutiche ed Alimentari, Via
       Brigata Salerno (Ponte), Genoa, I-16147, Italy
SO   Chemometrics and Intelligent Laboratory Systems (**1995**), 27(2), 189-203
AB   A procedure for the transfer of the **regression** equation in near-**IR**
       spectroscopy (**NIRS**), from a first instrument to a second instrument, is
       presented. The procedure uses partial least squares (PLS) **regression**
       twice: in the first step to compute the relationship between the spectra
       of transfer samples of the two instruments, and in the second step to
       compute the **regression** equation (relationship between chem. variables
       and spectral variables) of the first instrument. These two PLS steps
       are combined to predict the **regression** equation of the second
       instrument. Sometimes the PLS relationship between the two instruments
       is obtained from the principal components of the spectra of the two
       instruments. The procedure is applied to a set of 60 samples of soy
       flour, representative of the Italian soy prodn. 40 samples were used
       both as transfer samples and to compute the **regression** equation. 20
       samples were used as evaluation set. Spectra were recorded with four
       different instruments, in four different labs. The result of the
       transfer procedure were evaluated by means of the std. error of
       prediction (SEP) with the predicted **regression** equation. Owing also to
       the great no. of samples in the transfer set, and to the noise filtering
       effect of the twin PLS procedure, SEP with the predicted **regression**
       equation is not greater than that with the **regression** equation computed
       directly from the second instrument. The effect of some parameters,
       such as the no. of PLS latent variables in the two steps, is also
       studied.

L18   ANSWER 166 OF 226   CA   COPYRIGHT 2007 ACS on STN
AN   115:246824   CA
TI   **Multivariate** instrument standardization
AU   Wang, Yongdong; Veltkamp, David J.; Kowalski, Bruce R.
CS   Cent. Process Anal. Chem., Univ. Washington, Seattle, WA, 98195, USA
SO   Analytical Chemistry (**1991**), 63(23), 2750-6
AB   Three closely related problems assocd. with using **multivariate**
       calibration methods in spectroscopy have surfaced recently. The first
       problem involves the desire to transport a calibration model developed
       on one instrument to a second or even **multiple instruments**. Differences
       between the primary and secondary instruments which can occur for a
       variety of reasons can lead to erroneous results thereby prohibiting
       transferring the **calibration model** and necessitating the transport of
       the calibration samples. The second problem occurs when instruments

change over time (e.g. wavelength shift) for any reason. Again, using a calibration model for anal. when the instrument responses are altered after the time calibration was performed is problematic. The third problem is caused by the variation between samples from prodn. batches. The calibration model built from one batch might not be applicable to another batch. Using the mathematics of **multivariate** calibration, four different approaches to solving these two problems have been derived and tested with computer simulation. The four standardization methods proceed by acquiring the spectra of a well-chosen subset of the calibration samples and then either correcting the primary calibration model for use on secondary instruments or correcting the spectra acquired on the secondary instrument to account for the response differences. While standardization does not outperform using the entire calibration set for recalibration, only a 1.2-1.6 times larger error is obtained by standardization in the simulations and a study of a near-**IR** data set.

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